Quantum Dynamics by Solving Probabilistic Differential Equations via Autoregressive Networks

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Abstract

Quantum mechanics is fundamental to modern science and technology. Given the high dimensional nature of quantum mechanics, simulating quantum systems requires a large amount of computational power, which demands algorithms to efficiently approximate such systems. In this work, we apply an exact transformation that maps quantum dynamics to classical probabilistic differential equations. We then parameterize the probability distribution with autoregressive neural networks, which allows us to design efficient stochastic algorithms to simulate quantum evolution and solve for steady-state solutions.

Quantum Dynamics as Probabilistic Differential Equation

Open System Dynamics: Lindblad master equation[1]:

$$\frac{\partial \rho}{\partial t}(t) = \mathcal{L}[\rho(t)]$$

- ρ: density matrix (positive semi-definite and trace-one)
- $\mathcal{L}$: Liouvillian (linear) superoperator (depends on the system)

Probabilistic Differential Equation : First order differential equation:

$$\frac{\partial p_t}{\partial t}(a_1, a_2, \cdots, a_N) = \sum_{b_1, b_2, \cdots, b_N} p_t(b_1, b_2, \cdots, b_N) L^{b_1, b_2, \cdots b_N}_{a_1, a_2, \cdots a_N}$$

- p_t: a time dependent probability distribution over multiple qubits $a_i \in \{0,1,2,3\}$
- L: a $4^N \times 4^N$ matrix

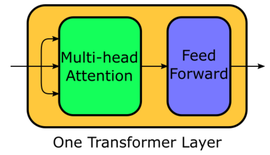
Quantum Classical Mapping:

- Positive operator-valued measure (POVM) operators[2, 3, 4]:
  - Frame:
    $$\{M_{(\boldsymbol{a})}\} = \{M_{(a_1)} \otimes M_{(a_2)} \otimes \cdots \otimes M_{(a_N)}\}$$
    - $M_{(a_i)}$: four 2×2 positive semidefinite matrices with $\sum_{(a_i)} M_{(a_i)} = \mathbb{I}$
  - Dual-frame:
    $$\{N^{(\boldsymbol{b})}\} = \{N^{(b_1)} \otimes N^{(b_1)} \otimes \cdots \otimes N^{(b_N)}\}$$
    - $N^{(b_i)}$: four 2×2 Hermitian matrices
- Probability distribution from density matrix
  $$p_t(\boldsymbol{a}) = \mathrm{Tr}\left(\rho M_{(\boldsymbol{a})}\right)$$
- Matrix coefficient of L from system Hamiltonian and dissipation

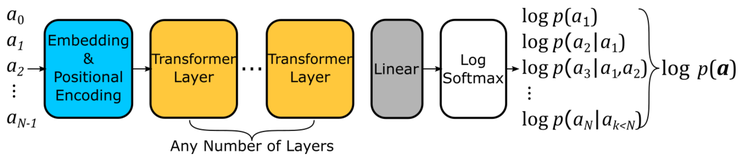
$$L^{\boldsymbol{b}}_{\boldsymbol{a}} = -i\,\mathrm{Tr}\left(\mathcal{H}\left[N^{(\boldsymbol{b})}, M_{(\boldsymbol{a})}\right]\right) + \sum_k \frac{\gamma_k}{2} \mathrm{Tr}\left(2\Gamma_k N^{(\boldsymbol{b})} \Gamma_k^\dagger M_{(\boldsymbol{a})} - \Gamma_k^\dagger \Gamma_k \{N^{(\boldsymbol{b})}, M_{(\boldsymbol{a})}\}\right)$$

  - $[\cdot,\cdot]$: commutator
  - $\{\cdot,\cdot\}$: anticommutator
  - $\mathcal{H} = J \sum_{\langle i,j \rangle} \sigma_i^{(z)} \sigma_j^{(z)} + h \sum_k \sigma_k^{(x)}$: system (transverse Ising) Hamiltonian
    - $\sigma_i^{(\alpha)}$: Pauli matrices
    - $\langle \cdot,\cdot \rangle$: neighboring sites
  - $\Gamma_k = \sigma_k^{(-)} = \frac{1}{2}\left(\sigma_k^{(x)} - i\sigma_k^{(y)}\right)$: jump (dissipation) operators

Autoregressive Transformer[5] Parameterization



- Parameterize
  $$p_\theta(\boldsymbol{a}) = \prod_k p_\theta(a_k | a_1, a_2, \cdots, a_{k-1})$$
- Exact sampling
  $$a_i \sim p_\theta(a_i | a_1, a_2, \cdots, a_{i-1})$$



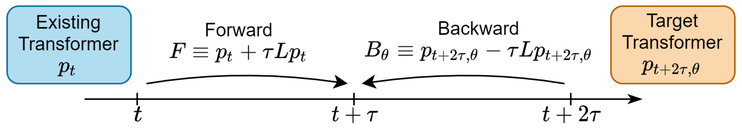
Dynamics Loss Function

Forward-Backward Trapezoid Method:

- Initialize $p_{(t=0),\theta}$
- At each time step with step size τ
  - Existing Transformer p_t
  - Target Transformer $p_{t+2\tau,\theta}$
  - Match p_t and $p_{t+2\tau,\theta}$ at $t+\tau$ stochastically with the cost function

$$\mathcal{C} = \frac{1}{N_s} \sum_{\boldsymbol{a} \sim p_{t+2\tau}}^{N_s} \frac{1}{p_{t+2\tau}(\boldsymbol{a})} \left| \sum_{\boldsymbol{b}} \underbrace{p_{t+2\tau,\theta}(\boldsymbol{b})\left(\delta^{\boldsymbol{b}}_{\boldsymbol{a}} - \tau L^{\boldsymbol{b}}_{\boldsymbol{a}}\right)}_{\text{Backward}} - \underbrace{p_t(\boldsymbol{b})\left(\delta^{\boldsymbol{b}}_{\boldsymbol{a}} + \tau L^{\boldsymbol{b}}_{\boldsymbol{a}}\right)}_{\text{Forward}} \right|$$

$$\theta = \arg\min E_{a \sim p_{t+2\tau}} \left[\frac{1}{p_{t+2\tau}(a)} |B_\theta(a) - F(a)| \right]$$



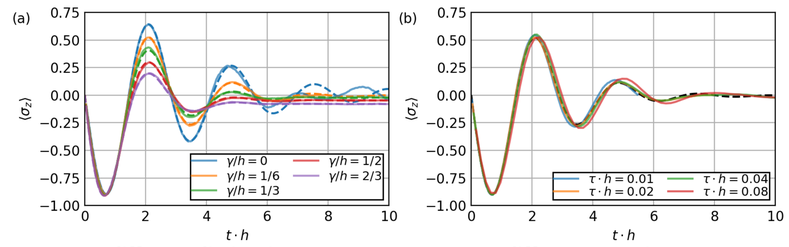
Steady-state Variational Method:

- For dissipative systems ($\gamma > 0$), a steady state is reached as $t \to \infty$
- Stochastically minimizing

$$\left\| \frac{\partial p}{\partial t} \right\|_1 \approx \frac{1}{N_s} \sum_{a \sim p}^{N_s} \frac{\sum_{\boldsymbol{b}} p_\theta(\boldsymbol{b}) L^{\boldsymbol{b}}_{\boldsymbol{a}}}{p(\boldsymbol{a})}$$

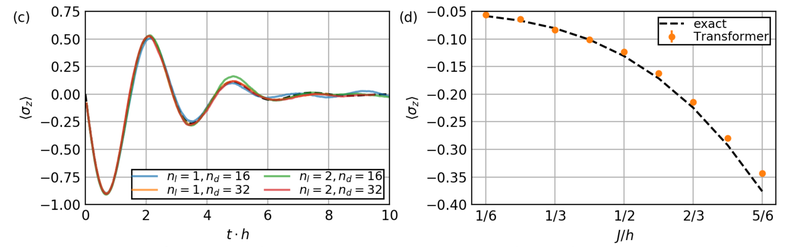
yields the same result as $p_{(t\to\infty),\theta}$

Experimental Results



Compare different dissipations:
Larger dissipation corresponds to stronger coupling to the environment and faster decohering of quantum effects. The smaller the dissipation, the quicker there is a deviation between the exact results and the Transformer results.

Compare different step sizes:
The errors mainly affect the frequency of the oscillation at larger times. The general shape is correct for different values of step sizes



Compare Transformer architectures:
Using different number of layers or hidden dimensions has small effect on the results, presumably because the bottleneck in the quality of our algorithm is not related to the representability, but the accumulated errors from imperfect optimizations.

Variational steady state:
The observable in the limit of large time using the variational approach. We find good agreement for theses fixed-points from the exact solution.

Conclusions

- Closely resemble the exact result for a 10-qubit transverse Ising model.
- Offer the probability to scale to larger systems.
- Broad applications for density matrix evolution in different contexts.
- Demonstrate how to approximately solve, using autoregressive neural networks, a high-dimensional probabilistic differential equation, which appears in a wide variety of classical contexts.

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